

4H-Pyran-4-one, tetrahydro-3,5-bis(hydroxymethyl)-  
67845-26-5 | DTXSID3028342

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

## Model Results

**Predicted value:** 5.31 days

**Global applicability domain:** Outside

**Local applicability domain index:** 4.26e-01

**Confidence level:** 8.64e-01

## Nearest Neighbors from the Training Set

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Propylbenzene

**Measured:** 24.3

**Predicted:** 4.02

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Ethylbenzene

**Measured:** 120

**Predicted:** 6.21

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4-Ethyltoluene

**Measured:** 24.3

**Predicted:** 3.95

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1,3-Diethylbenzene

**Measured:** 88.3

**Predicted:** 5.36

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1,2-Dimethyl-4-ethylbenzene

**Measured:** 40.7

**Predicted:** 4.08